



Fire and Combustion Research Programs at NSF

Phillip R. Westmoreland

Program Director, Combustion, Fire, and Plasma Systems (CFP)
Chemical, Bioengineering, Environmental, & Transport Systems CBET)
Directorate of Engineering
U.S. National Science Foundation
Arlington, VA 22230

NSF's focus is science with broad impacts.



- Official award criteria are:
 - (1) Intellectual merit -- Quality of the science.
 - (2) Broader impacts -- Technological, societal, educational.
- A significant sponsor of US academic research.
 - Science - not process or product development.
- Budget of about \$6 billion per year.
 - To double over the next ten years, based on the American Competitiveness Initiative.
- Operated as six broad directorates and six “offices,” the newest of which is the Office of Cyberinfrastructure.



NSF's interest: Combustion is a critical technology with far-reaching scientific demands.



- Classical combustion for energy and propulsion, augmented by heat transfer issues and tempered by need for pollution control.
- Exciting development in classical technologies, plus new technologies: microcombustors, catalytic combustors, material synthesis, cyberinfrastructure.
- At the same time, it has stimulated valuable science:
 - Computational chemistry (thermodynamics and kinetics)
 - Molecular-beam science
 - Laser diagnostics
 - Computational fluid dynamics and reactive-flow modeling



Combustion science at NSF is centered in the Engineering Directorate.



- My program, Combustion, Fire, and Plasma Systems, has a core budget about \$4.4 million per year.
 - Reactive CFD, chemistry, energetic materials, pollutants, fire and plasma materials synthesis, plasma ignition, plasma science.
- Funds about 35 investigator-initiated awards and 10 CAREER awards, plus conferences, undergraduate research support.
- A substantial additional amount of NSF support is by coordination of CFP with:
 - Other NSF programs (e.g., manufacturing, chemistry, international);
 - NSF and interagency initiatives (e.g., NSF-DOE Plasma Solicitation and the National Nanotechnology Initiative).



The other major NSF program for fire research is in “Structural Systems and Hazard Mitigation.”



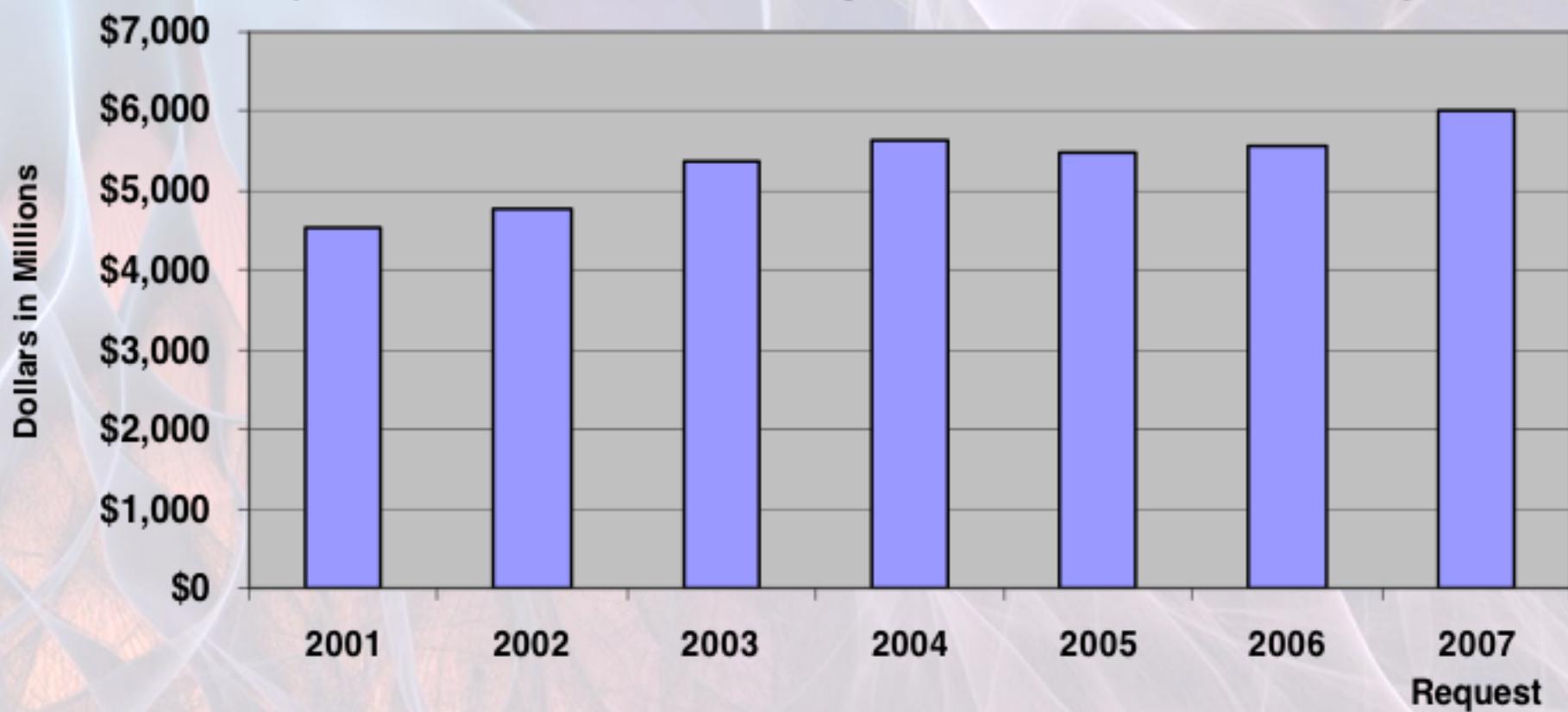
- Within ENG’s Division of Civil, Mechanical, and Manufacturing Innovation.
- Most of the resources and awards for fire research at NSF.
- Structures, structural elements, structural materials, and emergency systems.
- Total fire-research-related funding at NSF:
About \$2.9 million.



NSF Budget 2001-2007

FY 2007 Request \$6.02 billion

(+ \$439 million or 7.9 percent from FY 2006)



Congress & the White House agree: Increase needed in physical science & engineering.

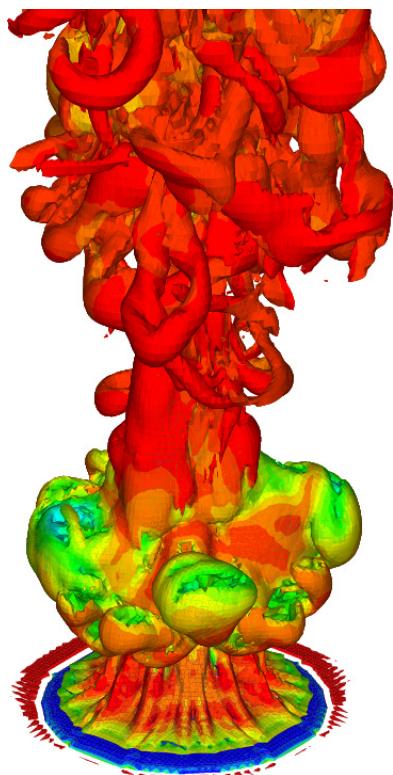


NATIONAL SCIENCE FOUNDATION

Examples:

High-Fidelity Numerical Modeling & Simulation of Fire Suppression

Paul E. DesJardin (U. Buffalo; CAREER Award, CTS-0348110)



- For suppressing pool fires, the P.I. predicts multiphase turbulent mixing processes over a wide range of time/length scales.
 - Turbulence modeling with reactions has been a grand-challenge problem.
 - Here, model large-scale turbulent motion directly by “Large-Eddy Simulation” method;
 - Model small scales stochastically; and
 - Account for interactions among nonlinear turbulence/chemistry/radiation/droplet models.
- Broad impacts are excellent: Researchers collaborate with Sandia, the Navy, & NIST.
- Supercomputer use for the 3-D calculations educates students about high-performance computing.

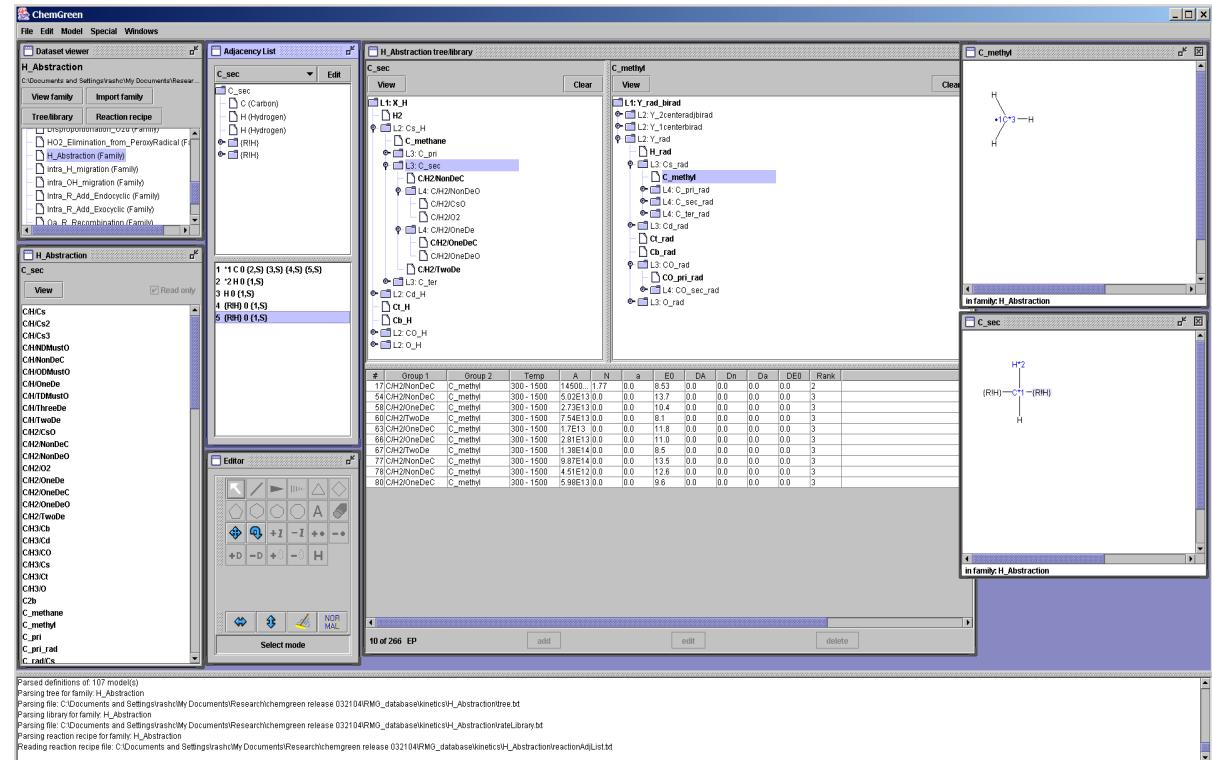




Automating Generation of Detailed Chemical Mechanisms

Bill Green (MIT) - CBET-0312359

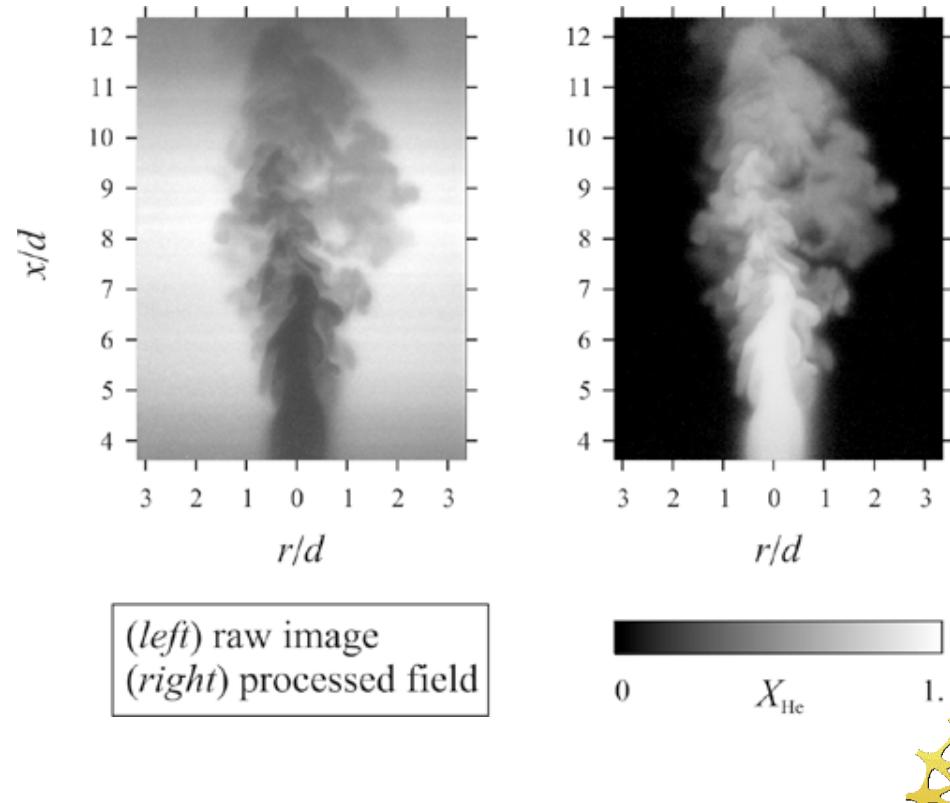
- Complicated chemical mechanisms abound in manufacturing, biology, environment, and energy & pollutants from combustion.
- Ultimately, they are sets of individual reactions.
- Project goal: To automate construction & solution of combustion simulations.
 - With XML data formats, maintain a large software package, used / modified by many researchers.
 - Include unambiguous documentation of simulation assumptions.
 - Generate simulation confidence limits along with the predictions.



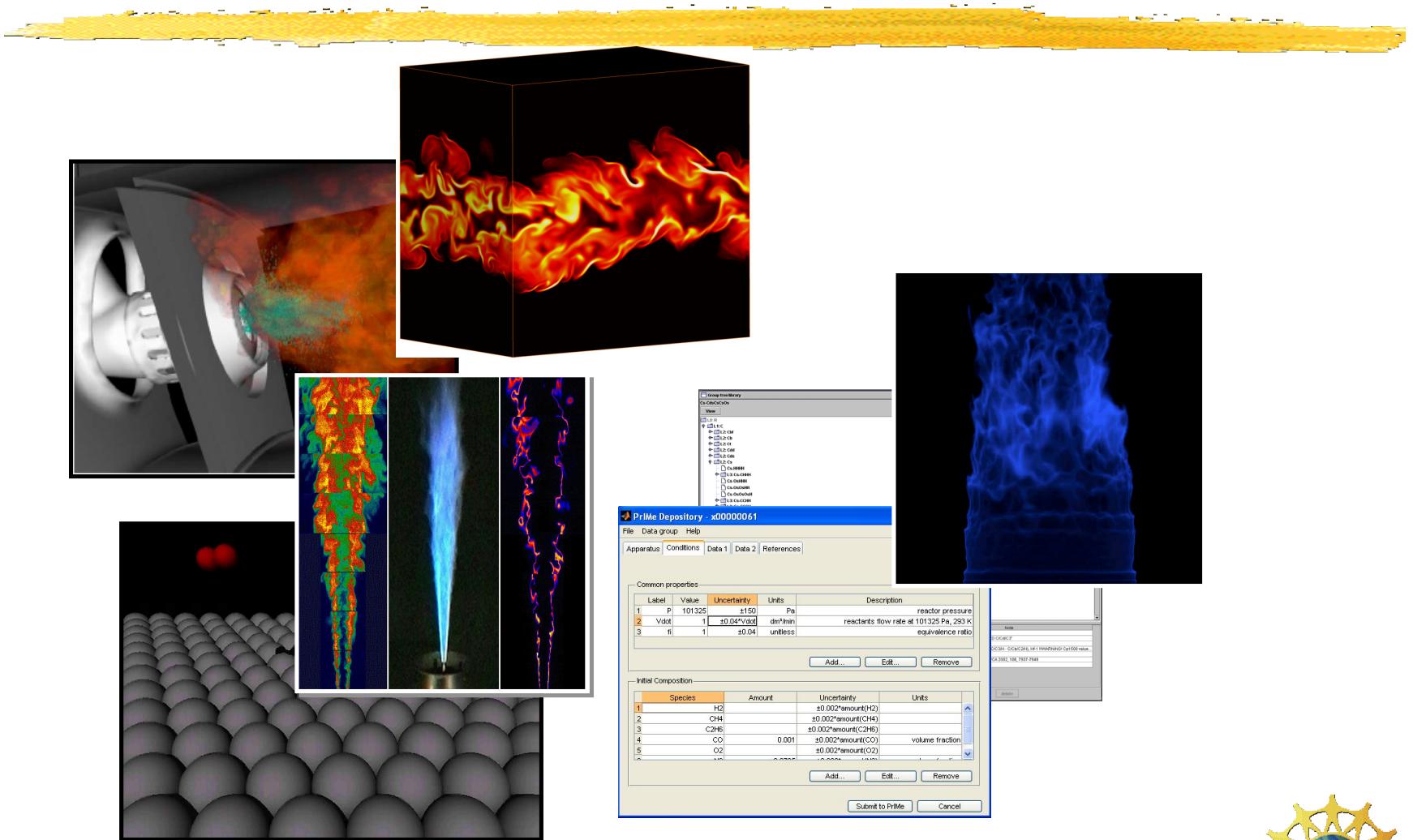
Crucial element of success: Close experimental interplay with simulation.

- Measurements of Subgrid-Scale Scalar Mixing to Study Large-Eddy Simulation of Turbulent Combustion
 - *Chenning Tong, Clemson U.*

- Application-Driven Combustion and Fluid Flow Imaging
 - *Lester Su,
Johns Hopkins U.*



Combustion research has been a leader in using cyber resources for modeling.



“Cyberinfrastructure” is a natural theme for us.



- Computers, networks, and their use.
- As in nanotechnology, we have been working in the field long before its recent definition.
 - Computer, code, and network development and use.
 - NSF Supercomputing Centers.
 - DOE SCIDAC program and CMCS.org
 - DoD High-Performance Computing Challenge Projects.
- Defining it as a concept opens new opportunities.



How do we best use it?



TeraGrid: Integrating NSF Cyberinfrastructure



TeraGrid is a facility that integrates computational, information, and analysis resources at the San Diego Supercomputer Center, the Texas Advanced Computing Center, the University of Chicago / Argonne National Laboratory, the National Center for Supercomputing Applications, Purdue University, Indiana University, Oak Ridge National Laboratory, the Pittsburgh Supercomputing Center, and the National Center for Atmospheric Research.

Charlie Catlett (ceo@uchicago.edu)

June 2006



- More powerful computing:
 - Grid computing
 - “Simulation-Based Engineering and Science”
 - “Cyber-Enabled Discovery and Innovation”
- Different ways of collecting data.
 - Remote sensor networks.
 - Remote experiments.
- More effective collaboration and information transfer:
 - “Virtual organizations” (gateways, collaboratories).



Virtual Organizations (VOs) can couple all three.



- Created by a group whose members and resources may be dispersed globally, yet who function as a coherent unit through the use of cyberinfrastructure.
- Extend beyond small collaborations and individual departments to encompass wide-ranging activities and groups.
- Provide shared access to centralized or distributed resources, such as community-specific sets of tools, applications, data, and sensors, and experimental operations, often in real time.
- In combustion research, two significant examples are:
 - Turbulent Nonpremixed Flame workshops (unsponsored),
www.ca.sandia.gov/TNF
 - PrIMe (NSF Chemistry sponsorship), prime.berkeley.edu



INTERNATIONAL WORKSHOP

ON MEASUREMENT AND COMPUTATION OF TURBULENT NONPREMIXED FLAMES

WORKSHOP ABSTRACT

EXPERIMENTAL DATA ARCHIVES

COMPUTATIONAL SUBMODELS

WORKSHOP PROCEEDINGS

RELATED INTERNET SITES

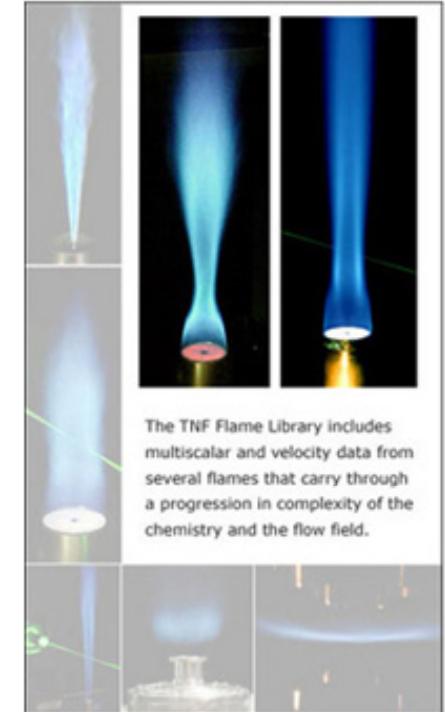
BIBLIOGRAPHY

ERRATA

TNF Workshop Abstract

This workshop is an open and ongoing international collaboration among experimental and computational researchers in turbulent nonpremixed and partially premixed combustion. The current emphasis is on fundamental issues of turbulence-chemistry interactions in gaseous flames. The objectives are to:

- Establish an internet library of well-documented flames that are appropriate for model validation and the advancement of basic scientific understanding of turbulent combustion.
- Provide a framework for collaborative comparisons of measured and modeled results.
- Identify priorities for further experimental and computational research.



The TNF Flame Library includes multiscalar and velocity data from several flames that carry through a progression in complexity of the chemistry and the flow field.

The TNF library includes multiscalar and velocity data from several flows and flames that carry through a progression in complexity of the chemistry and the flow field. Having started with simple jet flames of

PrIME Navigation

- [Home](#)
- [Announcements](#)
- [Calendar](#)
- **About PrIME**
 - [History](#)
 - [Organization](#)
 - [Documents](#)
 - [Membership](#)
 - [Technical Support](#)
 - [Website Support](#)
- [PrIME Data](#)
- [PrIME Codes](#)

Navigation

- [Applications](#)
- [groups](#)

Member Area

[Log in](#) | [Not a Member?](#)

Home

About PrIME

PrIME—Process Informatics Model—is a new approach for developing predictive models of chemical reaction systems that is based on the scientific collaborative paradigm and takes full advantage of existing and developing cyber infrastructure. The primary goals of PrIME are collecting and storing data, validating the data and quantifying uncertainties, and assembling the data into predictive models with quantified uncertainties to meet specific user requirements. The principal components of PrIME include: a data [Depository](#), which is a repository of data provided by the community, a data [Library](#) for storage of evaluated data, and a set of computer-based tools to process data and to assemble data into predictive models. Two guiding principles of PrIME are: [*open membership*](#)—a qualified individual or industrial organization can register to participate in the project; and [*open source*](#)—all submitted data, tools and models will be in the public domain.

»





an NCN project

Home my nanoHUB Resources Contributors Events About Support

Search

Help!

Nanotechnology 101

Introduction to nanotechnology



Nanotechnology 101 is a series of lectures designed to provide an undergraduate level introduction to nanotechnology. Our Nanotechnology 501 series offers lectures directed at the graduate student/ professional level.

[Learn more ▶](#)



[Simulate](#)

[Research](#)

[Teach & Learn](#)

[Contribute](#)

Annual Fire Conference, NIST Gaithersburg MD, April 4-5, 2007

Relevant new solicitation: Engineering Virtual Organizations (EVO)



Solicitation 07-558 issued April 4, 2006

Deadline for Letter of Intent: May 31, 2007

Deadline for Full Proposal: July 3, 2007, 5 p.m.
proposer's local time.



Two-year seed grants, up to \$200,000.



- Must establish an engineering virtual organization, enabled by CI, potentially including international participants.
- Must deploy its prototype EVO implementation
- Must create a conceptual design of its full implementation, drawing upon:
 - Articulated research and education goals of a research community to advance new frontiers.
 - Advances made by other scientific and engineering fields in establishing and operating VOs and their associated CI.
 - Commercially available CI tools and services.
 - CI tools and services emerging from current federal investments.



In summary, to reach our our goals:
Measure, monitor, analyze, predict, understand.



- For NSF, combustion and fire research cover a broad range of topics.
- In these complex systems, data are essential.
- Cyberinfrastructure tools will play an increasing role in database creation and use, including raw-data archiving.
- The approach of developing Virtual Organizations can be a powerful component of using CI.

